Project 28b
Combustion model development and validation

Stanford University

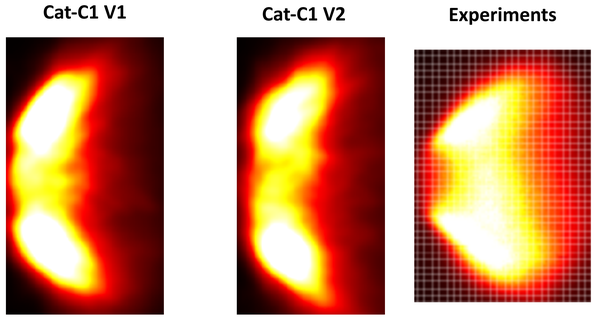
Motivation and Objectives

Reliable Computational Fluid Dynamics (CFD) simulation tools are required for the alternative fuels certification process:

- Development and evaluation of combustion model for high-fidelity simulations to characterize fuel effects in gas turbines
- High chemical fidelity necessary for predicting: **Lean-blow out/Altitude relight/Cold start**

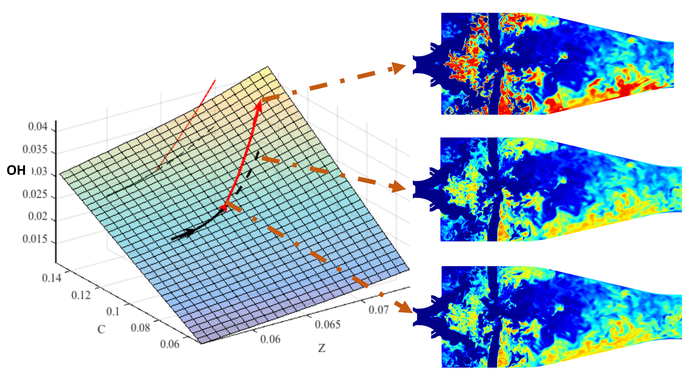
Impact of Finite-Rate Chemistry in LES

Tabulated chemistry model (e.g. FPV-model) shows low sensitivity with respect to the underlying kinetics schemes



Comparison of averaged OH* predicted by FPV-model with two versions of Cat-C1 HyChem schemes from FAA-Area 2

Compliance between a tabulated chemistry model (e.g. FPV-model) and underlying flow filed can be quantified via combustion-manifold analysis. Large deviation can often be found in complex configurations.

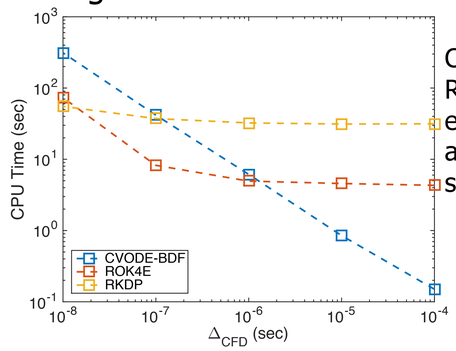


Deviation of finite-rate chemistry prediction of OH from the FPV tabulated chemistry value

Efficient Finite-Rate Chemistry

Semi-explicit Rosenbrock-Krylov schemes for stiff chemistry **ROK4E** :

- Explicit-like cost (linear in space & time)
- Non-iterative, high arithmetic density
- High order of accuracy
- 7 right-hand-side evaluations per step



Comparison of ROK4E with fully explicit (RKDP) and fully implicit schemes (CVODE)

Load balance issues in detailed kinetics calculations:

- Non-uniform chemical activity in space
  - number of ODE steps
  - number of active reactions/species
- Under-utilization of scalability

- Load rebalancing for distributed memory parallelization:
  -> distributed algorithm for the calculation of rebalancing partition
  -> non-blocking communication for work load sharing
- Rebalancing overhead is less than 1.5% with sharing work load of 80%
  (i.e. 80% of calculations performed by non-local processors)

Lead investigator: M. Ihme, Stanford University
Research Team: H. Wu, Q. Wang, J. Labahn, P. Ma
Project manager: Aniel Jardines and Cecilia Shaw, FAA;
Jeff Moder, NASA

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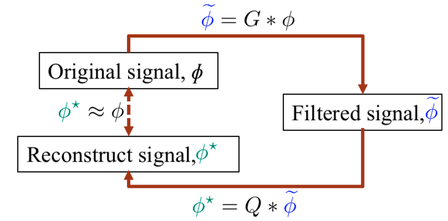
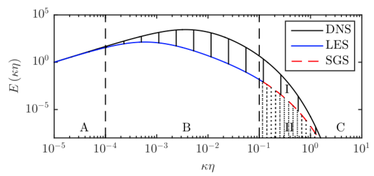
Generic Turbulent Combustion Model

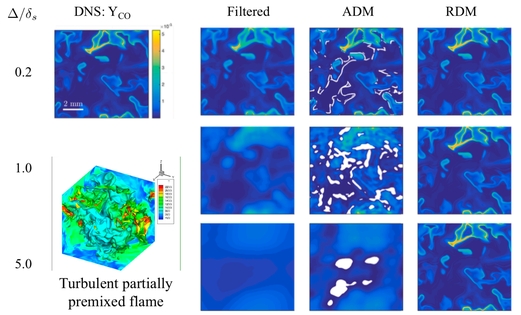
Deconvolution-based formulation for sub-grid closure

- Applicable to reactive LES regardless of the combustion model

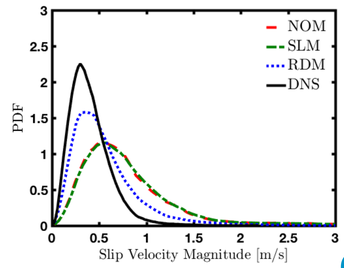




Regularized deconvolution method (**RDM**):
recovery of unfiltered signal while preserving important physical properties (boundedness, conservation, etc.)



Comparison of reconstructed scalar field by regularized (RDM) and un-regularized (ADM) deconvolution methods



Application of RDM to spray-combustion: Comparison of droplet sub-grid dispersion modeled by implicit model (NOM), simplified Langevin model (SLM), and regularized deconvolution method (RDM)

Conclusion

- Efficient calculation of finite-rate chemistry developed and implemented in state-of-art LES code
- Deconvolution based turbulent combustion model for both finite-rate and tabulated chemistry

Next Steps

- Adaptive integration of multiple combustion models (PEC) in unstructured compressible LES solver

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